

Dimethyl glutarate
1119-40-0 | DTXSID3025122

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 21.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.85e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

[Image not found](#)

N-Methyl-N'-phenylurea

Measured: 19.5

Predicted: 29.8

[Image not found](#)

Urea, 1-(p-fluorophenyl)-

Measured: 33.1

Predicted: 49.6

[Image not found](#)

1-Methoxy-2-propyl acetate

Measured: 2.29

Predicted: 7.33

[Image not found](#)

Urea, (3-methylphenyl)-

Measured: 36.3

Predicted: 37.2

[Image not found](#)

N-(3-chlorophenyl)-N'-methylurea

Measured: 85.1

Predicted: 101